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HIGHER ORDER TERMS IN THE MAGNETIC INTERACTION OF AN ION IN A S--ETC(U)

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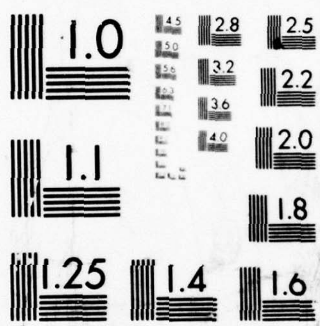

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The interaction Hamiltonian of an electron on an ion in the presence of a magnetic dipole is derived. This interaction is then cast into unit spherical tensor form for the N electron configuration $(n\ell)^N$. The lowest term in the interaction is shown to be the conventional term used in an effective internal field approximation. The remaining terms of the interaction can cause term dependent splitting of a magnetic impurity.

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APPENDICES

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1. INTRODUCTION

Recently, a number of papers have discussed ferromagnetic and antiferromagnetic phases of ionic solids containing a rare earth element as one of the major constituents.[1-4] In one of these papers,[1] a second rare earth is intentionally substituted in a small percentage to be used as a probe to investigate the internal fields in these solids at temperatures below the phase transition. The data were analyzed on the assumption of an effective magnetic field inside the sample. It was found that no single value of the effective field could be chosen to fit the Zeeman splitting observed on the substituted impurity ion.

In some of the papers, the experimental data were interpreted in terms of an effective magnetic field derived from a sum of the magnetic dipoles taken over the lattice. We show that these terms are only the lowest order of a particular multipolar expansion caused by the inclusion of the finite extent of the 4f electrons of the rare earth ions.

In this report, we first derive a convenient form for the interaction Hamiltonian of an orbital electron in the presence of a remote dipole and then cast this interaction into irreducible tensor form. The single-electron matrix elements are calculated, and the results are used to cast the interaction into unit spherical tensor form for the N electron configuration $(n\ell)^N$. The coefficients of the unit spherical tensors are shown to be particular lattice sums intimately related to those obtained in the point charge model of Stark splitting of ions in a crystal.

2. FUNDAMENTAL INTERACTION

2.1 Magnetic Dipole Field

We are concerned here with the effect of an inhomogeneous magnetic field due to external dipoles on the energy levels of a paramagnetic ion. Thus, we are led to consider the fundamental interaction between an electron and an inhomogeneous magnetic field. In this report, the sources of the inhomogeneous field may be considered pure dipoles.

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[1] *Donald Jean Randazzo, PhD Thesis, Johns Hopkins University, Baltimore, MD (1966) (University Microfilms, Ann Arbor, MI, No. 66-12,514).*

[2] *P. J. Becker, M. J. M. Leask, and R. N. Tyte, J. Phys. C, 5 (1972), 2027.*

[3] *J. C. Wright and H. W. Moos, Phys. Lett., 29A (1969), 495.*

[4] *H. G. Kahle, L. Klein, G. Müller-Voght, and H. C. Schopper, Phys. Status Solidi (b), 44 (1971), 619.*

The magnetic field at the point $\vec{r}$ due to a dipole of moment $\vec{M}$ situated at the point $\vec{R}$ is given by[5]

$$\vec{H} = \frac{3[\vec{M}\cdot(\vec{R}-\vec{r})]\,(\vec{R}-\vec{r})}{|\vec{R}-\vec{r}|^5} - \frac{\vec{M}}{|\vec{R}-\vec{r}|^3} . \tag{1}$$

It is well known that the magnetic vector potential corresponding to such a field is given by[5]

$$\vec{A} = -\frac{\vec{M}\times(\vec{R}-\vec{r})}{|\vec{R}-\vec{r}|^3} . \tag{2}$$

This vector potential may be written in the form*

$$\vec{A} = -[\vec{M}\times \text{grad}\,\phi(\vec{r})], \tag{3}$$

where

$$\phi(\vec{r}) = \frac{1}{|\vec{R}-\vec{r}|} . \tag{4}$$

Equation (4) may be expanded in spherical tensors:

$$\phi(\vec{r}) = \sum_{k,q} \frac{r^k}{R^{k+1}} C^\dagger_{kq}(\hat{R})\, C_{kq}(\hat{r}), \tag{5}$$

where

$$C_{kq}(\hat{r}) = \sqrt{\frac{4\pi}{2k+1}}\; Y_{kq}(\hat{r}) \tag{6}$$

and where Y_{kq} is the ordinary spherical harmonic.[6]

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[5] *W. K. H. Panofsky and M. Phillips, Classical Electricity and Magnetism, Addison Wesley, Reading, MA (1955), 127-128.*

[6] *M. E. Rose, Elementary Theory of Angular Momentum, John Wiley and Sons, Inc., New York (1957).*

**Here and in what follows, we use the notations "grad," "curl," etc., to represent an operator acting on only the function directly on the right of the operator, whereas the operator "∇" acts on everything to the right. For example,*

$$\nabla\phi = (\text{grad}\,\phi) + \phi\nabla .$$

Here the problem is to determine the interaction between a paramagnetic ion and a lattice of dipoles. Thus, we must sum the fields of equation (1) over all dipoles in the lattice. Here, we make our most crucial assumption: that the moments of all the paramagnetic ions in the lattice are equal; we allow for the possibility that the signs might vary, to allow for an antiferromagnetic lattice. With this assumption, we may use equation (3) for the vector potential, where $\phi(\vec{r})$ is now given by

$$\phi(\vec{r}) = \sum_{k,q} N^{\dagger}_{kq} \, C_{kq}(\hat{r}) \, r^{k}, \tag{7}$$

where

$$N_{kq} = \sum_{\substack{\text{paramagnetic} \\ \text{ions}}} \frac{(-)^{P_i} C_{kq}(\hat{R}_i)}{(R_i)^{k+1}} \tag{8}$$

and where the factor $(-)^{P_i}$ is considered to take account of the variation in sign of the dipoles. The quantities N_{kq} are called the magnetic crystal field parameters, by analogy with similar quantities which occur in considering the interaction of ions with the inhomogeneous electric field of crystal lattices.[7]

2.2 Correct Expression for Interaction

The expression for the interaction between an electron and a magnetic field is[8]

$$H_M = \frac{e}{2m}(\vec{p} \cdot \vec{A} + \vec{A} \cdot \vec{p}) + \frac{e\hbar}{mc}(\vec{\nabla} \cdot \text{curl } \vec{A}). \tag{9}$$

If into equation (9) we substitute equation (3) for the vector potential, taking account of the fact that the divergence of $\vec{A}$ is zero, we find that

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[7] *N. Karayianis and C. A. Morrison, Rare Earth Ion-Host Interactions 1. Point Charge Lattice Sum in Scheelites, Harry Diamond Laboratories TR-1648 (October 1973).*

[8] *L. I. Schiff, Quantum Mechanics, 3rd ed., McGraw-Hill Book Co., New York (1968), 478.*

$$H_M = 2\mu_B \, [i\vec{M} \cdot (\text{grad } \phi(\vec{r}) \times \vec{\nabla}) + (\vec{M} \cdot \text{grad}) \, (\vec{s} \cdot \text{grad } \phi(\vec{r}))] \, . \quad (10)$$

In equation (10), $\mu_B = e\hbar/2mc$, and $\vec{M}$ is the dipole moment of an external dipole. The quantity $\vec{s}$ is the spin angular momentum operator of the electron.

We now cast equation (10) into irreducible tensor form.[6]

3. IRREDUCIBLE TENSOR FORM OF H_M

We shall not consider the full interaction Hamiltonian of equation (10), but rather we shall break it into portions according to the decomposition of equation (7). Thus, equation (10) becomes

$$H_M = \sum_{k,q} N^{\dagger}_{kq} \, H_{kq} \, , \quad (11)$$

where

$$H_{kq} = 2\mu_B \, [i\vec{M} \cdot (\text{grad } \phi_{kq} \times \vec{\nabla}) + (\vec{M} \cdot \text{grad})(\vec{s} \cdot \text{grad } \phi_{kq})] \quad (12)$$

and where

$$\phi_{kq} = r^k \, C_{kq} \, (\hat{r}) \, . \quad (13)$$

We now cast equation (12) into irreducible tensor form. Using equation (A-26) (app A), we find that the second term of equation (12) becomes

$$\begin{aligned} H_{kq}(\text{spin}) &= 2\mu_B \sum_{\mu,\nu} (-)^{\mu+\nu} \, M_{-\mu} s_{-\nu} (\text{grad})_\mu \, (\text{grad})_\nu \, \phi_{kq} \\ &= 2\mu_B \, [k(k-1)\,(2k-1)\,(2k-3)]^{\frac{1}{2}} \, r^{k-2} \\ &\quad \times \sum_{\mu,\nu} \langle k-2(q+\mu+\nu)1(-\mu)|k-1(q+\nu)\rangle\langle k-1(q+\nu)1(-\nu)|k(q)\rangle \\ &\quad \times C_{k-2,q+\mu+\nu} \, M_{-\mu} \, s_{-\nu} \quad . \quad (14) \end{aligned}$$

[6] *M. E. Rose, Elementary Theory of Angular Momentum, John Wiley and Sons, Inc., New York (1957).*

It is convenient to recast equation (14) into a form which reflects explicitly that it is a tensor of rank (k-1) in the total angular momentum space of the electron. It may be recast by recoupling its Clebsch-Gordan (C-G) coefficients in equation (14) according to equation (A-13) (app A):

$$\langle k\text{-}2\ (q+\mu+\nu)1(-\mu)|k\text{-}1(q+\nu)\rangle\langle k\text{-}1(q+\nu)1(-\nu)|k(q)\rangle$$

$$= (2k-1)\ W(1\ k\text{-}2\ k\ 1;\ k\text{-}1\ k\text{-}1)$$

$$\times \langle k\text{-}2(q+\mu+\nu)1(-\nu)|k\text{-}1(q+\mu)\rangle\langle k\text{-}1(q+\mu)1(-\mu)|k(q)\rangle\ . \qquad (15)$$

But

$$W(1\ k\text{-}2\ k\ 1;\ k-1\ k-1) = \frac{1}{2k-1}\ . \qquad (16)$$

Therefore, we may rewrite equation (14) as

$$H_{kq}(\text{spin}) = H_{kq}^{(1)}$$

$$= 2\mu_B\ [k(k-1)\ (2k-1)\ (2k-3)]^{1/2}\ r^{k-2}$$

$$\times \sum_{\mu,\nu} \langle k\text{-}2(q+\mu+\nu)1(-\nu)|k\text{-}1(q+\mu)\rangle\langle k\text{-}1(q+\mu)1(-\mu)|k(q)\rangle$$

$$\times\ C_{k-2,q+\mu+\nu}\ s_{-\nu}\ M_{-\mu}\ . \qquad (17)$$

Now the first term in equation (12) is considerably more difficult to reduce. We may write

$$H_{kq}(\text{orbit}) = 2^{3/2}\ \mu_B \sum_{\mu,\nu}\ (-)^{\mu}\ M_{-\mu}\ \langle 1(\nu)1(\mu-\nu)|1(\mu)\rangle$$

$$\times\ (\text{grad}\ \phi_{kq})_{\nu}\ \nabla_{\mu-\nu}$$

$$= 2^{3/2}\ \mu_B \sum_{\mu,\nu}\ (-)^{\mu}\ M_{\mu}\ \langle 1(\nu)1(\mu-\nu)|1(\mu)\rangle(\text{grad}\ \phi_{kq})_{\nu}$$

$$\times\ [C_{1,\mu-\nu}\ \frac{\partial}{\partial r} - \sqrt{2}\ \sum_{\lambda}\ \langle 1(\lambda)1(\mu-\nu-\lambda)|1(\mu-\nu)\rangle\ \frac{1}{r}\ C_{1\lambda}\ell_{\mu-\nu-\lambda}]. \qquad (18)$$

Using the gradient formula equation (A-26) (app A) in equation (18), we find, using equation (13) for (grad $\phi_{kq})\nu$,

$$H_{kq}(\text{orbit}) = 2^{3/2}(2k+1)\langle 1(0)\; k(0)|k-1(0)\rangle \mu_B \sum_{\mu,\nu} (-1)^{\mu} M_{-\mu}$$

$$\times \langle 1(\nu)\; 1(\mu-\nu)|1(\mu)\rangle \langle 1(\nu)\; k(q)|k-1(q+\nu)\rangle$$

$$\times C_{k-1,q+\nu}\, C_{1,\mu-\nu}\, r^{k-1} \frac{\partial}{\partial r} - 4(2k+1)\langle 1(0)k(0)|k-1(0)\rangle\, \mu_B$$

$$\times \sum_{\mu,\nu,\lambda} (-1)^{\mu} M_{-\mu} \langle 1(\nu)1(\mu-\nu)|1(\mu)\rangle\langle 1(\nu)k(q)|k-1(q+\nu)\rangle$$

$$\times \langle 1(\lambda)1(\mu-\nu-\lambda)|1(\mu-\nu)\rangle C_{k-1,q+\nu}\, C_{1\lambda}\, \ell_{\mu-\nu-\lambda}\, r^{k-2}. \qquad (19)$$

Thus, the orbit part of the interaction divides into two parts; we shall consider each part separately.

The first term in the interaction is

$$H_{kq}^{(2)} = 2^{3/2}\mu_B\,(2k+1)\langle 1(0)k(0)|k-1(0)\rangle \sum_{\mu,\nu} (-)^{\mu} M_{-\mu}$$

$$\times \langle 1(\nu)1(\mu-\nu)\; 1(\mu)\rangle\langle 1(\nu)k(q)|k-1(q+\nu)\rangle\; r^{k-1}$$

$$\times C_{k-1,q+\nu}\, C_{1,\mu-\nu} \frac{\partial}{\partial r} \qquad (20)$$

$$= 2^{3/2}\,\mu_B\,(2k+1)\langle 1(0)\; k(0)|k-1(0)\rangle$$

$$\times \sum_{k'} \langle k-1(0)1(0)|k'(0)\rangle \sum_{\mu,\nu} (-)^{\mu} M_{-\mu}$$

$$\times \langle 1(\nu)1(\mu-\nu)|1(\mu)\rangle\langle 1(\nu)k(q)|k-1(q+\nu)\rangle$$

$$\times \langle k-1(q+\nu)1(\mu-\nu)|k'(q+\mu)\rangle\, C_{k',q+\mu}\, r^{k-1} \frac{\partial}{\partial r}\,. \qquad (21)$$

By recoupling the last two coefficients and summing over ν, we obtain

$$H_{kq}^{(2)} = 2\mu_B \,[6\,(2k - 1)]^{\frac{1}{2}}\,(2k + 1)\langle 1(0)\; k(0)|k-1(0)\rangle$$

$$\times \langle k-1(0)1(0)|k(0)\rangle W(k1\;k1;\;1k-1)r^{k-1}\sum_{\mu}\langle k(q+\mu)1(-\mu)|k(q)\rangle$$

$$\times\, C_{k,q+\mu}M_{-\mu}\,\frac{\partial}{\partial r}\,. \tag{22}$$

Now when we evaluate the C-G and Racah coefficients of equation (22), we find

$$H_{kq}^{(2)} = 2\mu_B\,[k(k+1)]^{\frac{1}{2}}\,r^{k-1}\sum_{\mu}\langle k(q+\mu)\;1(-\mu)|k(q)\rangle\, C_{k,q+\mu}\;M_{-\mu}\,\frac{\partial}{\partial r}\;. \tag{23}$$

We now come to the third term in the Hamiltonian, the second term in equation (19). This may be written as

$$H_{kq}^{(3)} = -\,4\mu_B\,(2k + 1)r^{k-2}\langle 1(0)k(0)|k-1(0)\rangle \sum_{\mu,\nu,\lambda}(-)^{\mu}M_{-\mu}\langle 1(\nu)1(\mu-\nu)|1(\mu)\rangle$$

$$\times\,\langle 1(\mu)k(q)|k-1(q+\nu)\rangle\langle 1(\lambda)1(\mu-\nu-\lambda)|1(\mu-\nu)\rangle\, C_{k-1,q+\nu}\;C_{1\lambda}\,\ell_{\mu-\nu-\lambda}$$

$$= -4\mu_B(2k+1)\langle 1(0)k(0)|k-1(0)\rangle r^{k-2}\sum_{k'}\langle k-1(0)1(0)|k'(0)\rangle$$

$$\times\qquad \langle 1(\nu-\lambda)1(\mu-\nu+\lambda)|1(\mu)\rangle\langle 1(\nu-\lambda)k(q)|k-1(q+\nu-\lambda)\rangle$$

$$\times\,\langle 1(\lambda)1(\mu-\nu)|1(\mu-\nu+\lambda)\rangle\langle k-1(q+\nu-\lambda)1(\lambda)|k'(q+\nu)\rangle$$

$$\times\, C_{k',q+\nu}\,\ell_{\mu-\nu}(-)^{\mu}M_{-\mu}. \tag{24}$$

We may recouple the first two C-G coefficients and then the last two and, finally, sum over λ to obtain

$$H_{kq}^{(3)} = -12\mu_B[k(2k-1)]^{\frac{1}{2}}r^{k-2}\sum_{k',k''}(-)^{k'+k''}\;[(2k'+1)(2k''+1)]^{\frac{1}{2}}$$

$$\times\, W(1\;1\;k-1\;k';1k'')W(1\;1\;k-1\;k';\;1k'')\,\langle k''(q+\mu)1(-\mu)|k(q)\rangle$$

$$\times\,\langle k'(q+\nu)1(\mu-\nu)|k''(q+\mu)\rangle\langle k-1(0)1(0)|k'(0)\rangle$$

$$\times\, C_{k',q+\nu}\;\ell_{\mu-\nu}M_{-\mu}\;. \tag{25}$$

We now repeat the expression for H_{kq} in irreducible tensor form:

$$H_{kq} = H_{kq}^{(1)} + H_{kq}^{(2)} + H_{kq}^{(3)} , \tag{26}$$

where

$$H_{kq}^{(1)} = 2\mu_B[k(k-1)(2k-1)(2k-3)]^{\frac{1}{2}} r^{k-2} \sum_{\mu,\nu} \langle k-2(q+\mu+\nu)1(-\nu)|k-1(q+\mu)\rangle$$
$$\times \langle k-1(q+\mu)1(-\mu)|k(q)\rangle C_{k-2,q+\mu+\nu} s_{-\nu} M_{-\mu} , \tag{27}$$

$$H_{kq}^{(2)} = 2\mu_B[k(k+1)]^{\frac{1}{2}} r^{k-1} \sum_{\mu} \langle k(q+\mu)1(-\mu)|k(q)\rangle C_{k,q+\mu} M_{-\mu} \frac{\partial}{\partial r} , \tag{28}$$

$$H_{kq}^{(3)} = -12\mu_B[(k(2k-1)]^{\frac{1}{2}} r^{k-2} \sum_{k',k''} (-)^{k'+k''} [(2k'+1)(2k''+1)]^{\frac{1}{2}}$$
$$\times W(1\ 1\ k\text{-}1k;\ 1k'')W(1\ 1\ k\text{-}1k';\ 1k'')\langle k-1(0)1(0)|k'(0)\rangle$$
$$\times \sum_{\mu,\nu} \langle k'(q+\nu)1(\mu-\nu)|k''(q+\mu)\rangle\langle k''(q+\mu)1(-\mu)|k(q)\rangle$$
$$\times M_{-\mu} C_{k',q+\nu} \ell_{\mu-\nu} . \tag{29}$$

4. SINGLE ELECTRON MATRIX ELEMENTS

We consider matrix elements of the operators of equations (27) to (29) between wave functions of the form

$$|n\ell m_\ell s m_s\rangle = \frac{R_{n\ell}(r)}{r} Y_{\ell m_\ell}(\theta_r, \phi_r)\, \chi(m_s) \tag{30}$$

with

$$\chi^\dagger(m'_s)\, \chi(m_s) = \delta_{m_s m'_s} . \tag{31}$$

First of all, we note that, if $n=n'$ and $\ell=\ell'$, the matrix elements of equation (28) may be integrated by parts over the radial variable to obtain

$$H_{kq}^{(2)} = -\mu_B(k + 1)\,[k(k + 1)]^{\frac{1}{2}}\langle r^{k-2}\rangle \sum_{\mu} \langle k(q+\mu)1(-\mu)|k(q)\rangle$$

$$\times\; C_{k,q+\mu}\, M_{-\mu}\;. \qquad (32)$$

Thus, according to the Wigner-Eckart theorem, we obtain for the matrix elements of $H_{kq}^{(2)}$

$$\langle \ell m_\ell ' s\, m_s'|H_{kq}^{(2)}|\ell m_\ell\; s m_s\rangle = -\mu_B\;(k + 1)[k(k + 1)]^{\frac{1}{2}}\, \langle r^{k-2}\rangle\, \delta_{m_s m_s'}$$

$$\langle \ell||C_k||\ell\rangle \sum_{\mu} M_{-\mu} \langle k(q+\mu)1(-\mu)|k(q)\rangle\langle \ell(m_\ell)k(q + \mu)|\ell(m_\ell ')\rangle, \qquad (33)$$

where

$$\langle r^k\rangle = \int_0^\infty dr\; r^k|R_{n\ell}(r)|^2. \qquad (34)$$

The quantity $\langle \ell||C_k||\ell\rangle$ is the reduced matrix element of C_{kq} (app B).

The matrix elements of $H_{kq}^{(3)}$ are

$$\langle \ell m_\ell ' s\; m_s '|H_{\ell q}^{(3)}|\ell m_\ell s\; m_s\rangle = -12\mu_B[k(2k-1)]^{\frac{1}{2}}\langle r^{k-2}\rangle\delta m_s m_s'$$

$$\times \sum_{k',k''} (-)^{k'+k''}[\ell(\ell+1)(2k'+1)(2k''+1)]^{\frac{1}{2}}\langle \ell||C_k '||\ell\rangle\, \langle k\text{-}1(0)1(0)|k'(0)\rangle$$

$$\times\; W(1\;1\;k\text{-}1k\;;1k'')\; W(1\;1\;k\text{-}1k';\;1k'') \sum_{\mu,\nu} \langle k'(q+\nu)1(\mu-\nu)|k''(q+\mu)\rangle$$

$$\times\; \langle k''(q+\mu)1(-\mu)|k(q)\rangle\, \langle \ell(m_\ell)1(\mu-\nu)|\ell(m_\ell+\mu-\nu)\rangle$$

$$\times\; \langle \ell(m_\ell+\mu-\nu)\;\; k'(q+\nu)|\ell(m_\ell ')\rangle. \qquad (35)$$

We may recouple[6] the last two C-G coefficients of equation (34) and sum on ν to obtain

$$<\ell m_\ell' s\ m_s|H_{kq}^{(3)}|\ell m_\ell s\ m_s> = 12\mu_B[k(2k-1)\ell(\ell+1)(2\ell+1)]^{\frac{1}{2}}<r^{k-2}>$$

$$\times\ \delta_{m_s m_s'} \sum_{k',k''} (2k''+1)\sqrt{(2k'+1)}<k-1(0)1(0)|k'(0)> \quad .$$

$$\times\ W(\ell 1\ell k';\ell k'')W(1\ 1\ k\text{-}1k\ ;1k'')W(1\ 1\ k\text{-}1k';\ 1k'')<\ell||C_k'||\ell>$$

$$\times \sum_\mu M_{-\mu}<\ell(m_\ell)k''(q+\mu)|\ell(m_\ell')><k''(q+\mu)1(-\mu)|k(q)>. \tag{36}$$

To determine the behavior of equation (35), we must examine each term separately. The quantity of interest in our analysis is

$$t(k,k',k'') = (2k''+1)[k(2k-1)(2k'+1)\ell(\ell+1)(2\ell+1)]^{\frac{1}{2}}<k-1(0)1(0)|k'(0)>$$

$$\times\ W(\ell 1\ell k';\ell k'')W(1\ 1\ k\text{-}1k;\ 1k'')W(1\ 1\ k\text{-}1k';1k'')<\ell||C_k||\ell>. \tag{37}$$

By evaluating explicitly the quantities occurring in equation (37) according to equation (A-17) (app A),

$$t(k,\ k,\ k) = \frac{1}{12}\ (k + 1)\ \sqrt{k(k + 1)}\ <\ell||C_k||\ell>\ , \tag{38}$$

$$t(k,\ k,\ k\text{-}1) = -\ \frac{(k - 1)}{12}\ \left[\frac{k(2\ell - k + 1)(2\ell + k + 1)}{(2k - 1)}\right]^{\frac{1}{2}}\ <\ell||C_k||\ell>\ , \tag{39}$$

$$t(k,\ k - 2,\ k - 1) = -\ \frac{k}{12}\ \left[\frac{k(2\ell - k + 1)(2\ell + k + 1)}{(2k - 1)}\right]^{\frac{1}{2}}\ <\ell||C_k||\ell>\ , \tag{40}$$

where we have used the equation.

$$<\ell||C_{k-2}||\ell> = -\ (\frac{k}{k-1})\ \left[\frac{(2\ell + k + 1)(2\ell - k + 1)}{(2\ell + k)\ (2\ell - k + 2)}\right]^{\frac{1}{2}}\ <\ell||C_k||\ell>. \tag{41}$$

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[6]*M. E. Rose, Elementary Theory of Angular Momentum, John Wiley and Sons, Inc., New York (1957).*

Therefore, the total of equation (36) is

$$<\ell m_\ell' s m_s'|H_{kq}^{(3)}|\ell m_\ell\ s m_s> = \mu_B(k+1)\sqrt{k(k+1)}\ <r^{k-2}>\delta_{m_s m_s'}\ <\ell||C_k||\ell>$$

$$\times \sum_\mu M_{-\mu} <\ell(m_\ell)k(q+\mu)|\ell(m_\ell')><k(q+\mu)1(-\mu)|k(q)>$$

$$-\mu_B[k(2k-1)(2\ell-k+1)(2\ell+k+1)]^{\frac{1}{2}}\ <r^{k-2}>\delta_{m_s m_s'}\ <\ell||C_k||\ell>$$

$$\times \sum_\mu M_{-\mu}<\ell(m_\ell)k-1(q+\mu)|\ell(m_\ell')><k-1(q+\mu)1(-\mu)|k(q)>. \qquad (42)$$

The first term of equation (42) cancels equation (33) exactly, and therefore we have

$$<\ell m_\ell' s\ m_s'|H_{kq}^{(2)}+H_{kq}^{(3)}|\ell m_\ell s\ m_s> = -\ \mu_B[k(2k-1)(2\ell-k+1)(2\ell+k+1)]^{\frac{1}{2}}$$

$$\times\ <r^{k-2}>\delta_{m_s m_s'}\ <\ell||C_k||\ell>\sum_\mu M_{-\mu}<\ell(m_\ell)k-1(q+\mu)|\ell(m_\ell')>$$

$$\times\ <k-1(q+\mu)1(-\mu)|k(q)>\ . \qquad (43)$$

Finally, for the spin part, we have

$$<\ell m_s' s\ m_s'|H_{kq}^{(1)}|\ell m_\ell s m_s> = 2\mu_B[k(k-1)(2k-1)(2k-3)s(s+1)]^{\frac{1}{2}}<\ell||C_{k-2}||\ell>$$

$$\times\ <r^{k-2}>\ \sum_{\mu,\nu} M_{-\mu}<k-2(q+\mu+\nu)1(-\nu)|k-1(q+\mu)>\ <k-1(q+\mu)1(-\mu)|k(q)>$$

$$\times\ <\ell(m_\ell)k-2(q+\mu+\nu)|\ell(m_\ell')><s(m_s)1(-\nu)|s(m_s')>\ . \qquad (44)$$

5. MATRIX ELEMENTS FOR EQUIVALENT ELECTRONS

We now consider the problem of N electrons, each with orbital angular momentum ℓ. We introduce the unit tensors[9] u_q^k and $v_{\lambda q}^{1k}$, which are defined such that

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[9] *G. Racah, Phys. Rev., 62 (1942), 438.*

$$<\ell's'||u^k||\ell s> = \delta_{\ell\ell'}\,\delta_{ss'} \tag{45}$$

and

$$<\ell's'||v^{1k}||\ell s> = \delta_{\ell\ell'}\,\delta_{ss'}\,. \tag{46}$$

The quantity u^k is a tensor of rank k in orbital space; v^{1k} is a double tensor of rank k in orbital space and rank 1 in spin space. We may write the Hamiltonian equations (27) to (29) in a form using the unit tensors:

$$H_{kq}^{(1)} = 2\mu_B[k(2k-1)(2k-3)(k-1)s(s+1)]^{\frac{1}{2}}<\ell||C_{k-2}||\ell><r^{k-2}>$$

$$\times \sum_{\mu,\nu} M_{-\mu}\, v^{1,k-2}_{-\nu,q+\mu+\nu} <k-2(q+\mu+\nu)1(-\nu)|k-1(q+\mu)>$$

$$\times <k-1(q+\mu)1(-\mu)|k(q)>, \tag{47}$$

$$H_{kq}^{(2')} = -\mu_B[k(2k-1)(2\ell-k+1)(2\ell+k+1)]^{\frac{1}{2}}<\ell||C_k||\ell><r^{k-2}>$$

$$\times \sum_{\mu} M_{-\mu}\, u^{k-1}_{q+\mu}<k-1(q+\mu)1(-\mu)|k(q)>, \tag{48}$$

with

$$H_{kq} = H_{kq}^{(1)} + H_{kq}^{(2')}\,. \tag{49}$$

When we go over to N equivalent electrons, we sum the one-electron Hamiltonian equation (49) over all N electrons. We define the unit tensors for N electrons as the sum over all the one-electron tensors:

$$U_q^k = \sum_{i=1}^{N} u_q^k(i), \tag{50}$$

$$V_{\lambda q}^{1k} = \sum_{i=1}^{N} v_{\lambda q}^{1k}\,(i). \tag{51}$$

Therefore the Hamiltonian for N equivalent electrons becomes

$$H_{kq}(N) = H_{kq}^{(1)} + H_{kq}^{(2')} , \tag{52}$$

where

$$H_{kq}^{(1)} = 2\mu_B \; [k(k-1)(2k-1)(2k-3)s(s+1)]^{\frac{1}{2}} \langle \ell || C_{k-2} || \ell \rangle \langle r^{k-2} \rangle$$

$$\times \sum_{\mu,\nu} M_{-\mu} \; V^{1,k-2}_{-\nu,q+\mu+\nu} \langle k-2(q+\mu+\nu)1(-\nu)|k-1(q+\mu)\rangle$$

$$\times \langle k-1(q+\mu)1(-\mu)|k(q)\rangle \tag{53}$$

and where

$$H_{kq}^{(2')} = -\mu_B \; [k(2k-1)(2\ell-k+1)(2\ell+k+1)]^{\frac{1}{2}} \langle \ell || C_k || \ell \rangle \langle r^{k-2} \rangle$$

$$\times \sum_{\mu} M_{-\mu} \; U^{k-1}_{q+\mu} \; \langle k-1(q+\mu)1(-\mu)|k(q)\rangle . \tag{54}$$

When matrix elements are taken of equations (54) and (53), they are expressed in terms of the C-G coefficients and reduced matrix elements of the unit tensors. In particular, in a basis $|JMLS\rangle$, where L is the total orbital angular momentum, S is the total spin angular momentum, and $\vec{J} = \vec{L} + \vec{S}$, we have

$$\langle \alpha' J' M' L' S' | H_{kq}^{(1)} | \alpha JMLS \rangle = 2\mu_B [k(k-1)(2k-1)(2k-3)\, s(s+1)]^{\frac{1}{2}} \langle \ell || C_{k-2} || \ell \rangle$$

$$\times \langle r^{k-2} \rangle \langle \alpha' L' S' || V^{1,k-2} || \alpha LS \rangle [(2s+1)(2S'+1)(2L'+1)(2k-1)]^{\frac{1}{2}}$$

$$\times X(SLJ;\; S'L'J';\; 1\; k-2\; k-1) \sum_{\mu} \langle k-1(q+\mu)1(-\mu)|k(q)\rangle$$

$$\times \langle J(M)k-1(q+\mu)|J'(M')\rangle \; M_{-\mu} \tag{55}$$

for the spin part of the interaction and

$$\langle\alpha'J'M'L'S'|H_{kq}^{(2')}|\alpha SMLS\rangle = -\mu_B[k(2k-1)(2\ell-k+1)(2\ell+k+1)]^{\frac{1}{2}} \langle\ell||C_k||\ell\rangle$$

$$\times \langle r^{k-2}\rangle\langle\alpha'L'S'||U^{k-1}||\alpha LS\rangle[(2L'+1)(2J+1)]^{\frac{1}{2}} \delta_{SS'} W(k-1\ L'J\ S;\ L\ J')$$

$$\times \sum_{\mu} \langle k-1(q+\mu)(-\mu)|k(q)\rangle\langle J(M)k-1(q+\mu)|J'(M')\rangle M_{-\mu} . \tag{56}$$

The quantities α and α' in equations (55) and (56) are additional quantum numbers necessary to uniquely identify the states. The quantity X(abc;def;ghi) is the X-coefficient and is identical to a 9-J symbol. The manipulations necessary for the results in equations (55) and (56) are given in appendix B. The quantities $\langle\alpha'L'S'||U^{k-1}||\alpha LS\rangle$ and $\langle\alpha'L'S'||V^{1,k-2}||\alpha LS\rangle$ are reduced matrix elements of the unit tensors in the Russell-Saunders basis and are tabulated extensively.[10]

6. OPERATOR EQUIVALENT FOR LOWEST TERM

We now consider the k = 2 part of the Hamiltonian equations (47) and (48). Substituting the explicit form

$$\langle\ell||C_2||\ell\rangle = \langle\ell(0)2(0)|\ell(0)\rangle = -\left[\frac{\ell(\ell+1)}{(2\ell+3)(2\ell-1)}\right]^{\frac{1}{2}} , \tag{57}$$

the Hamiltonian becomes

$$H_{2q} = \mu_B\ \sqrt{6} \sum_{\mu} M_{-\mu}\ (\ell_{q+\mu} + 2s_{q+\mu})\ \langle 1(q+\mu)1(-\mu)|2(q)\rangle . \tag{58}$$

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[10]*C. W. Nielson and George F. Koster, Spectroscopic Coefficients for the p^n, d^n, and f^n Configurations, The MIT Press, Cambridge, MA (1963). The relations between the reduced matrix elements used in that book and in our report are*

$$\langle\alpha'L'S'||U^k||\alpha LS\rangle = \left[\frac{2\ell+1}{2L'+1}\right]^{\frac{1}{2}} (\alpha'L'S'||U^k||\alpha LS)$$

and

$$\langle\alpha'L'S'||V^{1k}||\alpha LS\rangle = \frac{2}{\sqrt{3}} \left[\frac{2\ell+1}{(2L'+1)(2S'+1)}\right]^{\frac{1}{2}} (\alpha'L'S'||V^{1k}||\alpha LS).$$

We now prove that this equation is identical to the usual Hamiltonian for a constant magnetic field:

$$H = \mu_B (\vec{\ell} + 2\vec{s}) \cdot \vec{H}. \tag{59}$$

We consider a single term,

$$\phi_{kq} = C_{kq} r^k , \tag{60}$$

and calculate the field according to equation (3):

$$H_\mu = -[\vec{\nabla}\times(\vec{M}\times\vec{\nabla}\phi)]_\mu = 2\sum_{\nu\lambda} <1(\nu)1(\mu-\nu)|1(\mu)><1(\lambda)1(\mu-\nu-\lambda)|1(\mu-\nu)>$$

$$\times M_\lambda \nabla_\nu \nabla_{\mu-\nu-\lambda} C_{2q} r^2 = 30 M_{q+\mu} <1(0)2(0)|1(0)><1(0)1(0)|0(0)>$$

$$\times \sum_\nu <1(\nu)1(\mu-\nu)|1(\mu)><1(q+\mu)1(-q-\nu)|1(\mu-\nu)><1(-q-\nu)2(q)|1(-\nu)>$$

$$\times <1(\nu)1(-\nu)|0(0)> . \tag{61}$$

If we recouple the first two C-G coefficients and explicitly evaluate them with j = 0, we arrive at the result

$$H_\mu = (-)^\mu \sqrt{6}\, M_{q+\mu} <1(q+\mu)1(-\mu)|2(q)> . \tag{62}$$

This result, when substituted in equation (59), gives

$$H = \mu_B \sum_\mu (-)^\mu H_{-\mu} (\ell_\mu + 2s_\mu) , \tag{63}$$

which was to be proved.

7. DISCUSSION OF RESULTS

In view of the results of section 6, it is convenient to write the Hamiltonian as the sum of two terms:

$$H = \mu_B (\vec{L} + 2\vec{S}) \cdot \vec{H}_{eff} + \sum_{k>4,q} N_{kq}{}^\dagger H_{kq}, \tag{64}$$

where H_{kq} is given by equation (52) and the magnetic crystal field parameters, N_{kq}, are given by equation (8). The quantity H_{eff} is related to the twofold parameters N_{2q}.

Considering a ferromagnetic below its Curie point, we may assume that all the dipoles in the lattice are equal and pointing along the same direction. In particular, we assume a lattice whose point group symmetry is S_4; thus, the only nonzero magnetic crystal field parameters are N_{20}, N_{40}, N_{60}, N_{44}, and N_{64}. We assume the field points along the z-direction. If the material is insulating and there are several inert atoms between the paramagnetic ions, we may neglect the exchange interaction and assume that there is a pure dipole interaction. Under these conditions, we may assume the form of equation (64) for the Hamiltonian.

We consider the zero-field splitting of doublets by the Hamiltonian equation (64). Usually only the first term of equation (64) is taken into account; that is, it is assumed that the splitting of doublets in a ferromagnetic material is due to an effective magnetic field H_{eff}. However, experimentally it has been shown that a single effective field could not account for all the splittings observed (say, by optical methods or excited state electron paramagnetic resonance--EPR). The splittings can be accounted for if all the terms of equation (64) are considered. These terms represent the effect of the inhomogeneity of the magnetic field near the paramagnetic ion.

In conclusion, we have investigated the effect of a lattice of external dipoles on the energy levels of a paramagnetic ion. Consideration of such an effect may be represented by an effective Hamiltonian which is the sum of two terms; the first term representts the effects of a constant field, and the second term represents the effects of the inhomogeneity of the field. No attempt has been made to investigate fully the consequences of the Hamiltonian equation (64) for this report.

LITERATURE CITED

(1) Donald Jean Randazzo, PhD Thesis, Johns Hopkins University, Baltimore, MD (1966) (University Microfilms, Ann Arbor, MI, No. 66-12,514).

(2) P. J. Becker, M. J. M. Leask, and R. N. Tyte, J. Phys. C, 5 (1972), 2027.

(3) J. C. Wright and H. W. Moos, Phys. Lett., 29A (1969), 495.

(4) H. G. Kahle, L. Klein, G. Müller-Voght, and H. C. Schopper, Phys. Status Solidi (b), 44 (1971), 619.

(5) W. K. H. Panofsky and M. Phillips, Classical Electricity and Magnetism, Addison Wesley, Reading, MA (1955), 127-128.

(6) M. E. Rose, Elementary Theory of Angular Momentum, John Wiley and Sons, Inc., New York (1957).

(7) N. Karayianis and C. A. Morrison, Rare Earth Ion-Host Interactions 1. Point Charge Lattice Sum in Scheelites, Harry Diamond Laboratories TR-1648 (October 1973).

(8) L. I. Schiff, Quantum Mechanics, 3rd ed., McGraw-Hill Book Co., New York (1968), 478.

(9) G. Racah, Phys. Rev., 62 (1942), 438.

(10) C. W. Nielson and George F. Koster, Spectroscopic Coefficients for the p^n, d^n, and f^n Configurations, The MIT Press, Cambridge, MA (1963).

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APPENDIX A.--CLEBSCH-GORDAN COEFFICIENTS AND RACAH COEFFICIENTS

A-1. CLEBSCH-GORDAN COEFFICIENTS

The Clebsch-Gordan (C-G) coefficients are defined through the relation

$$|j_1 j_2 jm\rangle = \sum_{m_1 m_2} \langle j_1(m_1) j_2(m_2)|j(m)\rangle |j_1 m_1 j_2 m_2\rangle , \qquad \text{(A-1)}$$

which describes the coupling of two angular momenta $\vec{j}_1$ and $\vec{j}_2$ to form a sum $\vec{j}$. The C-G coefficient,

$$\langle j_1(m_1) j_2(m_2)|j(m)\rangle ,$$

is zero unless $m_1 + m_2 = m$ and unless $|j_1 - j_2| \leq j \leq |j_1 + j_2|$. The sum $j_1 + j_2 + j$ must be an integer.

Certain symmetry equations relate different C-G coefficients:

$$\langle j_1(m_1) j_2(m_2)|j(m)\rangle = (-)^{j_1+j_2-j} \langle j_2(m_2) j_1(m_1)|j(m)\rangle \qquad \text{(A-2)}$$

$$= (-)^{j_1+j_2-j} \langle j_1(-m_1) j_2(-m_2)|j(-m)\rangle \qquad \text{(A-3)}$$

$$= (-)^{j_1-m_1} \left[\frac{2j+1}{2j_2+1}\right]^{1/2} \langle j_1(m_1) j(-m)|j_2(-m_2)\rangle \qquad \text{(A-4)}$$

$$= (-)^{j_2+m_2} \left[\frac{2j+1}{2j_1+1}\right] \langle j(-m) j_2(m_2)|j_1(-m_1)\rangle . \qquad \text{(A-5)}$$

A-2. RACAH COEFFICIENTS

In the coupling of three angular momenta, we consider two coupling schemes:

$$\text{Scheme A:} \quad \vec{j}_1 + \vec{j}_2 = \vec{j}_{12}, \ \vec{j}_{12} + \vec{j}_3 = \vec{j}, \qquad \text{(A-6)}$$

$$\text{Scheme B:} \quad \vec{j}_1 + \vec{j}_3 = \vec{j}_{13}, \ \vec{j}_{13} + \vec{j}_2 = \vec{j} . \qquad \text{(A-7)}$$

APPENDIX A

Coupling scheme A is represented by the wave function

$$|A\rangle = \sum_{m_1 m_2 m_3} \langle j_1(m_1) j_2(m_2) | j_{12}(m_1+m_2)\rangle \langle j_{12}(m_1+m_2) j_3(m_3) | j(m)\rangle \times |j_1 m_1 j_2 m_2 j_3 m_3\rangle \tag{A-8}$$

and scheme B by the wave function

$$|B\rangle = \sum_{m_1 m_2 m_3} \langle j_1(m_1) j_3(m_3) | j_{13}(m_1+m_3)\rangle \langle j_{13}(m_1+m_3) j_2(m_2) | j(m)\rangle \times |j_1 m_1 j_2 m_2 j_3 m_3\rangle . \tag{A-9}$$

The coupling schemes A and B are connected by a unitary transformation

$$|B\rangle = \sum_A \langle A|B\rangle \; |A\rangle , \tag{A-10}$$

and the coefficients of the unitary transformation are determined by taking the inner product of equation (A-8) with equation (A-9).

We define the Racah coefficients as follows:

$$W(j_1\; j_{12}\; j_{13}\; j_3;\; j_1\; j) = \frac{1}{[(2j_{12}+1)(2j_{13}+1)]^{\frac{1}{2}}} \langle A|B\rangle . \tag{A-11}$$

Thus,

$$\begin{aligned}
&[(2j_{12}+1)(2j_{13}+1)]^{\frac{1}{2}}\, W(j_2\; j_{12}\; j_{13}\; j_3;\; j_1\; j) \\
&= \sum_{m_1 m_2} \langle j_1(m_1) j_2(m_2) | j_{12}(m_1+m_2)\rangle \langle j_{12}(m_1+m_2) j_3(m-m_1-m_2) | j(m)\rangle \\
&\times \langle j_1(m_1) j_3(m-m_1-m_2) | j_{13}(m-m_2)\rangle \langle j_{13}(m-m_2) j_2(m_2) | j(m)\rangle .
\end{aligned} \tag{A-12}$$

The following equation can be obtained from equation (A-12):

$$\langle j_2(m_2)j_1(m_1)|j_{12}(m_1+m_2)\rangle\langle j_{12}(m_1+m_2)j_3(m-m_1-m_2)|j(m)\rangle$$

$$= \sum_{j_{13}} [(2j_{12}+1)(2j_{13}+1)]^{\frac{1}{2}} W(j_2 j_1 j\, j_3,\, j_{12} j_{13})$$

$$\times \langle j_1(m_1)j_3(m-m_1-m_2)|j_{13}(m-m_2)\rangle\langle j_2(m_2)j_{13}(m-m_2)|j(m)\rangle\ , \qquad \text{(A-13)}$$

which is a relationship used often in the main body of the report.

The Racah coefficient is related to the symmetrized "6j" symbol by the following equation:

$$W(abcd;\, ef) = (-)^{a+b+c+d} \begin{Bmatrix} a & b & e \\ d & c & f \end{Bmatrix}. \qquad \text{(A-14)}$$

Certain symmetry relations exist for the "6j" symbols:

$$\begin{Bmatrix} j_1 & j_2 & j_3 \\ \ell_1 & \ell_2 & \ell_3 \end{Bmatrix} = \begin{Bmatrix} j_2 & j_1 & j_3 \\ \ell_2 & \ell_1 & \ell_3 \end{Bmatrix} = \begin{Bmatrix} j_1 & j_3 & j_2 \\ \ell_1 & \ell_3 & \ell_2 \end{Bmatrix} = \begin{Bmatrix} j_1 & \ell_2 & \ell_3 \\ \ell_1 & j_2 & j_3 \end{Bmatrix} \qquad \text{(A-15)}$$

and all combinations of the relations in equation (A-11). The four triads $(j_1\ j_2\ j_3)$, $(j_1\ \ell_2\ \ell_3)$, $(\ell_1\ j_2\ \ell_3)$, and $(\ell_1\ \ell_2\ j_3)$ must be able to form a triangle. That is,

$$|j_1 - j_2| \le j_3 \le j_1 + j_2\ , \qquad \text{(A-16)}$$

with similar relations for the other triads. An explicit formula for the "6j" symbol is

$$\begin{Bmatrix} j_1 & j_2 & j_3 \\ \ell_1 & \ell_2 & \ell_3 \end{Bmatrix} = [\Delta(j_1 j_2 j_3)\Delta(j_1 \ell_2 \ell_3)\Delta(\ell_1 j_2 \ell_3)\Delta(\ell_1 \ell_2 j_3)]^{\frac{1}{2}}$$

$$\times \sum_t \frac{(-)^t\,(t+1)!}{(t-j_1-j_2-j_3)!(t-j_1-\ell_2-\ell_3)!(t-\ell_1-j_2-\ell_3)!(t-\ell_1-\ell_2-j_3)!}$$

$$\times \frac{1}{(j_1+j_2+\ell_1+\ell_2-t)!(j_1+j_3+\ell_1+\ell_3-t)!(j_2+j_3+\ell_2+\ell_3-t)!}\ , \qquad \text{(A-17)}$$

which is used in the main body of the report to evaluate explicitly certain "6j" symbols and Racah coefficients. In the above, t ranges over all values for which the arguments of the factorials are nonnegative integers. The quantity $\Delta(abc)$ is

$$\Delta(abc) = \frac{(a+b-c)!\,(a-b+c)!\,(-a+b+c)!}{(a+b+c+1)!} . \qquad \text{(A-18)}$$

Another relation which is used in the text is

$$\sum_x (-)^{a+b+c+d+e+f+g+j+h+x}(2x+1)\begin{Bmatrix} abx \\ cdg \end{Bmatrix}\begin{Bmatrix} cdx \\ efh \end{Bmatrix}\begin{Bmatrix} efx \\ baj \end{Bmatrix} = \begin{Bmatrix} ghj \\ ead \end{Bmatrix}\begin{Bmatrix} ghj \\ fbc \end{Bmatrix} . \qquad \text{(A-19)}$$

The X-coefficient or "9j" symbol, arising through consideration of the coupling of four angular momenta, is given in terms of "6j" symbols by

$$\begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j_4 & j_{34} \\ j_{13} & j_{24} & j \end{Bmatrix} = \sum_g (-)^{2g}(2g+1)\begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_{34} & j & g \end{Bmatrix}\begin{Bmatrix} j_3 & j_4 & j_{34} \\ j_2 & g & j_{24} \end{Bmatrix}\begin{Bmatrix} j_{13} & j_{24} & j \\ g & j_1 & j_3 \end{Bmatrix} . \qquad \text{(A-20)}$$

A-3. SOME USEFUL RELATIONS

It is useful to represent the dot and cross products of two vectors in the form

$$(\vec{A}\cdot\vec{B}) = \sum_\mu (-)^\mu A_\mu B_{-\mu} , \qquad \text{(A-21)}$$

$$(\vec{A}\times\vec{B})_\mu = -\sqrt{2}\, i \sum_\nu \langle 1(\nu)1(\mu-\nu)|1(\mu)\rangle A_\nu B_{\mu-\nu} , \qquad \text{(A-22)}$$

where

$$A_0 = A_z ,$$

$$A_1 = -\frac{1}{\sqrt{2}}(A_x + i A_y) ,$$

$$A_{-1} = \frac{1}{\sqrt{2}}(A_x - i A_y) . \qquad \text{(A-23)}$$

We list below some useful relations involving the manipulation of certain spherical tensors. First of all, a third spherical tensor can be formed from two others:

$$C_{k_1q_1}C_{k_2q_2} = \sum_{kq} \langle k_1(q_1)k_2(q_2)|k(q)\rangle\langle k_1(0)k_2(0)|k(0)\rangle\, C_{kq}\,. \qquad \text{(A-24)}$$

Second, a relation for the gradient of a radial function multiplied by a spherical tensor can be obtained:

$$(\text{grad})_\mu C_{kq} f(r) = \sum_{k'} \langle 1(\mu)k(q)|k'(q+\mu)\rangle\langle 1(0)k(0)|k'(0)\rangle C_{k',q+\mu}$$

$$\times \left[\frac{\partial f}{\partial r} + \frac{\sqrt{6}}{r} f(r)[k(k+1)(2k+1)]^{\frac{1}{2}}\, W(k1k'1;\, k1)\right]. \qquad \text{(A-25)}$$

If $f(r) = r^k$, equation (A-25) becomes

$$(\text{grad})_\mu C_{kq} r^k = (2k+1)\langle 1(\mu)k(q)|k-1(q+\mu)\rangle\langle 1(0)k(0)|k-1(0)\rangle C_{k-1,q+\mu} r^{k-1}$$

$$= -[k(2k+1)]^{\frac{1}{2}}\langle 1(\mu)k(q)|k-1(q+\mu)\rangle C_{k-1,q+\mu} r^{k-1}\,. \qquad \text{(A-26)}$$

If $f(r) = r^{-k-1}$, then equation (A-25) becomes

$$(\text{grad})_\mu\, f(r) C_{kq} = -[(k-1)(2k+1)]^{\frac{1}{2}}\langle 1(\mu)k(q)|k+1(q+\mu)\rangle \frac{C_{k+1,q+\mu}}{r^{k+2}}\,. \qquad \text{(A-27)}$$

APPENDIX B.--IRREDUCIBLE TENSORS

Irreducible tensor operators are defined as operators that have the same transformation properties under rotation as do the spherical harmonics. To express this definition concisely, we write the commutation relations of the spherical tensor T_{kq} and the components of the angular momentum

$$[J_\mu, T_{kq}] = \sqrt{k(k+1)}\ \langle k(q)\ 1(\mu)|k(q+\mu)\rangle\ T_{k,q+\mu} \quad , \qquad \text{(B-1)}$$

where $J_0 = J_z$, $J_1 = -1/\sqrt{2}\ (J_x + i\ J_y)$, and $J_{-1} = 1/\sqrt{2}\ (J_x - i\ J_y)$.

Equation (B-1) defines T_{kq} as an irreducible tensor operator of rank k and projection q.

The power of the irreducible tensor formalism lies in the ability to use the Wigner-Eckart (W-E) theorem to calculate matrix elements:

$$\langle J'M'|T_{kq}|JM\rangle = \langle J(M)\ k(q)|J'(M')\rangle\langle J'||T_k||J\rangle\ . \qquad \text{(B-2)}$$

This important theorem states that the dependence of the matrix element on the left of equation (B-2) on the projection q and the azimuthal quantum numbers M and M' is contained entirely in the Clebsch-Gordan (C-G) coefficient. The so-called "reduced matrix element," $\langle J'||T_k||J\rangle$, depends only on J', J, and k.

If $T_{k_1q_1}$ and $U_{k_2q_2}$ are irreducible tensors, then so is the quantity

$$V_{kq} = \sum_{q_1} T_{k_1q_1}\ U_{k_2,q-q_1}\ \langle k_1(q_1)k_2(q-q_1)|k(q)\rangle\ . \qquad \text{(B-3)}$$

This irreducibility may be shown by using the W-E theorem and the recoupling schemes of appendix A.

We now proceed to calculate reduced matrix elements of two types of irreducible tensors in a basis $|JMLS\rangle$: a tensor in L-space and a tensor in J-space.

For a tensor in L-space (that is, a quantity which satisfies equation (B-1) with $\vec{J}$ replaced by $\vec{L}$), we have, by the W-E theorem,

APPENDIX B

$$\langle J'M'L'S'|T_{kq}|JMLS\rangle = \sum_{M_L M_L'} \langle L(M_L)S(M-M_L)|J(M)\rangle$$

$$\times \langle L'(M_L')S'(M-M_L')|J'(M')\rangle \delta_{SS'} \delta_{M-M_L, M'-M_L'}$$

$$\times \langle L(M_L)k(q)|L'(M_L')\rangle \langle L||T_k||L\rangle , \quad \text{(B-4)}$$

where we have used the expansion

$$|JMLS\rangle = \sum_{M_L} \langle L(M_L)S(M-M_L)|J(M)\rangle |LM_L S, M-M_L\rangle . \quad \text{(B-5)}$$

If we eliminate the sum over M_L' by the Kronecker delta, recouple the last two C-G coefficients, and sum over M_L, we arrive at the result

$$\langle J'L'S'||T_k||JLS\rangle = [(2L'+1)(2J+1)]^{\frac{1}{2}} W(kL'JS'\ LJ') \langle L'||T_k||L\rangle . \quad \text{(B-6)}$$

For a tensor in J-space, we use the form of equation (B-3), where $T_{k^1q^1}$ operates in L-space, and $U_{k^2q^2}$ operates in S-space. Therefore, we have

$$\langle J'M'L'S'|V_{kq}|JMLS\rangle = \sum_{M_L M_L' q_1} \langle L(M_L)S(M-M_L)|J(M)\rangle$$

$$\times \langle L'(M_L')S'(M'-M_L')|J'(M')\rangle \langle k_1(q_1)k_2(q-q_1)|k(q)\rangle$$

$$\times \langle L(M_L)k_1(q_1)|L'(M_L')\rangle \langle S(M-M_L)k_2(q-q_1)|S'(M_L-M_L')\rangle$$

$$\times \langle L'||T_{k_1}||L\rangle \langle S'||U_{k_2}||S\rangle . \quad \text{(B-7)}$$

If we recouple the second and fifth C-G coefficients and the third and fourth C-G coefficients and sum over q_1, we obtain

$$<J'M'L'S'|V_{kq}|JMLS>=<L'||T_{k_1}||L><S'||U_{k_2}||S>(-)^{L'+S'-J'+k_1+k_2}$$

$$\times\sum_{M_L,g}(-)^{-g-M_L}[(2L'+1)(2S'+1)]^{\frac{1}{2}}(2g+1)W(Sk_2J'L';S'g)$$

$$\times\ W(LL'kk_2;k_1g)<S(M-M_L)g(M_L+q)|J'(M')>$$

$$\times\ <L(-M_L)g(M_L+q)|k(q)><L(M_L)S(M-M_L)|J(M)>\ . \qquad \text{(B-8)}$$

If we further recouple the first and second C-G coefficients in equation (B-8) and sum over M_L and q using equation (A-20) (app A), we arrive at the final result:

$$<J'L'S'||V_{kq}||JLS>\ =\ [(2L'+1)(2S'+1)(2s+1)(2k+1)]^{\frac{1}{2}}\begin{Bmatrix} L & S & J \\ k_1 & k_2 & k \\ L' & S' & J' \end{Bmatrix}$$

$$\times\ <L'||T_{k1}||L><S'||U_{k2}||S>\ . \qquad \text{(B-9)}$$

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